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**An experimental determination of the Debye–Waller temperature factor for nickel.** By M.J. COOPER and R.I. TAYLOR, *Materials Physics Division, A.E.R.E., Harwell, Berkshire, England*

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An accurate neutron diffraction study of a nickel powder sample has been carried out at three different wavelengths. Excellent agreement was found between the data obtained at the various wavelengths and a least-squares refinement gave a value for the Debye–Waller temperature factor,  $B_{Ni}$ , of  $0.426 (\pm 0.009) \text{ \AA}^2$  at room temperature ( $295^\circ\text{K}$ ).

An accurate neutron diffraction study of a nickel powder sample has been carried out at room temperature ( $295^\circ\text{K}$ ) on the new high resolution neutron powder diffractometer PANDA, which was installed recently at the Harwell PLUTO reactor. In view of the International Powder Intensity Project for comparing X-ray diffraction measurements from essentially identical samples of nickel powder (see Jennings, 1969) it was decided to use a sample from the same nickel powder as was used in this X-ray project, in case information from the neutron study might be of use in the interpretation of the X-ray measurements.

The sample was loosely packed into a 1 cm diameter vanadium container and measurements of the Bragg intensities were made at three different wavelengths, in order to investigate any wavelength or angle dependent effects which might not be apparent at a single wavelength. At each wavelength all reflexions were measured in such a way as to provide an integrated intensity with a standard deviation due to counting statistics alone of the order of 1% or less and measurement of the 111 reflexion was repeated at regular intervals to confirm the reliability of the relative measurements. An investigation of the scattering from the empty container confirmed the absence of any anomalous contributions from the container to the measured intensities and a linear background correction was made between points on either side of the Bragg peaks. Due to overlap between the scattering associated with the 311 and 222 reflexions there is some uncertainty in the background corrections for these and this is significant for the weaker 222 reflexion, particularly at the shortest wavelength. The standard deviation of the intensity of the 222 reflexion has therefore been increased to allow for this uncertainty. Corrections for the residual thermal diffuse scattering were calculated by the method of Chipman & Paskin (1959); these corrections were in all cases less than 1% of the Bragg intensity. Experimental structure factors ( $F_o$ ) were then calculated from the intensities and the values for the three

wavelengths were scaled together so that those of the reference (111) reflexion became equal. The scaled  $F_o$  values are listed in Table 1 together with their standard deviations, which, except for the 222 reflexion, are those based on counting statistics alone. It can be seen from the Table that there is excellent agreement between the data obtained at the various wavelengths.

Theoretical structure factors ( $F_c$ ) were calculated from a model with only the scale factor and the temperature factor ( $B_{Ni}$ ) as refinable parameters. The magnetic contribution to the structure factors, which is less than  $\frac{1}{2}\%$  for all reflexions, was calculated from the  $p/b$  values determined by Mook (1966), where  $p$  and  $b$  are, respectively, the magnetic and nuclear scattering amplitudes. A least-squares refinement was then carried out, comparing the calculated structure factors with the mean observed structure factors ( $\bar{F}_o$ ), weighted in accordance with the listed standard deviations. Because of the uncertainty associated with the 222 reflexion at  $0.8 \text{ \AA}$ , this measurement was not included in the determination of  $\bar{F}_o$ . The refinement gave an  $R$  value ( $= \Sigma(|\bar{F}_o| - |F_c|) / \Sigma|F_c|$ ) of  $0.32\%$  and a value of  $B_{Ni} = 0.426 (\pm 0.009) \text{ \AA}^2$ . The values of  $\bar{F}_o$  and  $F_c$  are also listed in Table 1.

Previous experimental values for  $B_{Ni}$  vary from  $0.25$  to  $0.50 \text{ \AA}^2$ , the most recent value being  $0.37 (\pm 0.02) \text{ \AA}^2$  (Inkinen & Suortti, 1964). However, in view of the doubt now cast upon the accuracy of such X-ray measurements (see Jennings, 1969) this value may be in question. In any case, one would expect to obtain a more reliable value from neutron measurements because of the small angular dependence of the scattering amplitude and the lesser importance of such factors as absorption and preferred orientation.

Barron & Smith (1966) have calculated a value for  $B_{Ni}$  of  $0.381 (\pm 0.008) \text{ \AA}^2$  from the phonon dispersion measurements of Birgeneau, Cordes, Dolling & Woods (1964). The value obtained in the present work is somewhat larger than this calculated value. However, it should be noted that the

Table 1. *Scaled neutron structure factors for nickel powder sample*

<i>hkl</i>	$\lambda = 0.8 \text{ \AA}$		$\lambda = 1.1 \text{ \AA}$		$\lambda = 1.5 \text{ \AA}^*$		Mean observed	Calculated
	$F_o$	$\sigma(F_o)$	$F_o$	$\sigma(F_o)$	$F_o$	$\sigma(F_o)$	$\bar{F}_o$	$F_c$
111	25.46	0.03	25.46	0.10	25.46	0.02	25.46	25.47
200	25.26	0.09	25.18	0.11	25.23	0.04	25.22	25.23
220	24.44	0.09	24.34	0.12	24.42	0.04	24.40	24.33
311	23.81	0.07	23.78	0.10	23.74	0.03	23.78	23.68
222	23.70†	0.50	23.36	0.30	23.38	0.08	23.37	23.46
400	22.37	0.04	22.55	0.13			22.46	22.67
331	22.13	0.02					22.13	22.09
420	21.91	0.02					21.91	21.91
422	21.05	0.03					21.05	21.17

\* A  $\lambda/2$  correction was made at this wavelength.

† Not included in calculation of  $\bar{F}_o$  (see text).

latter, although including anharmonic effects due to the expansion of the lattice, does not include anharmonic effects due to higher order terms in the interatomic potential (see Willis, 1969). Willis has estimated the increase in the temperature factors for KCl at 293°K, resulting from inclusion of these higher order terms, to be about 10%. The present result would therefore indicate that a similar increase occurs for nickel.

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**Symbolism of rhombohedral space groups in Miller axes.** By J. D. H. DONNAY, *The Johns Hopkins University, Baltimore, Maryland 21218, U. S. A.*

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The point symmetry of the hexagonal lattice,  $6/m\ 2/m\ 2/m$ , possesses 3 kinds of symmetry directions (*Blickrichtungen*); that of the rhombohedral lattice,  $\bar{3}\ 2/m$ , has only two. The proposed extension of the Hermann-Mauguin symbolism rests on this fact. Examples:  $P311 = P3$ ,  $P31 = R3$ . The dummy 1s stand for lattice-symmetry directions, as in the well-known symbols  $P3m1$ ,  $P31m$ , etc.

The question has been raised of the desirability of having a dual symbolism capable of representing the seven rhombohedral space groups both in the Bravais and in the Miller system of coordinate axes. At the present time *International Tables for X-ray Crystallography* use the same symbols:

$$R\bar{3}m, R\bar{3}c, R32, R3m, R3c, R\bar{3}, R3 \quad (1)$$

whether the cell used to describe the lattice is the triple ('*R* centered') hexagonal cell (*hR*) or the rhombohedral primitive cell (*rP*).

An extremely simple method of referring the space-group symbol to the *rP* cell is already available in the Hermann-Mauguin notation itself: use *P* instead of *R* as lattice letter and no confusion can result in 5 cases out of the 7 listed in (1). Indeed the symbols

$$P\bar{3}m, P\bar{3}c, P32, P3m, P3c \quad (2)$$

are new symbols, distinctly different from the hexagonal symbols

$$P\bar{3}m1, P\bar{3}1m; P\bar{3}c1, P\bar{3}1c; P321, P312; P3m1, P31m\ P3c1, P31c, \quad (3)$$

that apply to other space groups. In the symbols of the rhombohedral space groups (2), the lattice letter (*R* or *P*) is followed by two symmetry-element symbols, whereas in the hexagonal space-group symbols (3) the lattice letter *P* is followed by three. The notation reflects the fundamental fact that the point symmetry of the rhombohedral lattice,  $\bar{3}\ 2/m$ , contains one primary axis, three secondary axes, but no tertiary axes (such as are present in the symmetry  $6/m\ 2/m\ 2/m$  of the hexagonal lattice). In Carl Hermann's terminology the *Blickrichtungen* are of two kinds in a rhombohedral lattice and of three kinds in a hexagonal lattice, for it is obvious that the *Blickrichtungen* are the symmetry directions of the lattice.

Table 1. *Symbols of trigonal space groups*

Proposed new symbols and additions to old symbols are shown in bold face.

		$\bar{3}m1$	321	3m1	$\bar{3}11$	311
		$\bar{3}1m$	312	31m		
Hexagonal lattice (point symmetry $6/m\ 2/m\ 2/m$ )	Bravais axes <i>hP</i>	$P\bar{3}m1$	<b><i>P321</i></b>	<i>P3m1</i>	<b><i>P\bar{3}11</i></b>	<b><i>P311</i></b>
		<i>P\bar{3}1m</i>	<b><i>P312</i></b>	<i>P31m</i>		<b><i>P31,211</i></b>
			<b><i>P31,221</i></b>			
			<b><i>P31,212</i></b>			
		<b><i>P\bar{3}c1</i></b>	<i>P3c1</i>			
		<b><i>P\bar{3}1c</i></b>	<i>P31c</i>			
		$\bar{3}m$	32	3m	$\bar{3}1$	31
Rhombohedral lattice (point symmetry $\bar{3}2/m$ )	Bravais axes <i>hR</i>	<b><i>R\bar{3}m</i></b>	<b><i>R32</i></b>	<i>R3m</i>	<b><i>R\bar{3}</i></b>	<b><i>R3</i></b>
		<b><i>R\bar{3}c</i></b>		<i>R3c</i>		
	Miller axes <i>rP</i>	<b><i>P3m</i></b>	<b><i>P32</i></b>	<b><i>P3m</i></b>	<b><i>P31</i></b>	<b><i>P31</i></b>
		<b><i>P3c</i></b>		<b><i>P3c</i></b>		